

## CALCULATION SUPPORTING INFORMATION

### Isocanthine Synthesis via Rh(III)-Catalyzed Intramolecular C–H Functionalization

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### Computational Details

All the calculations were conducted with Gaussian 09 software.<sup>1</sup> The B3LYP functional<sup>2</sup> was used for the gas-phase geometry optimization of all species. The LANL2DZ basis set<sup>3</sup> was employed for Rh and Cu, and the 6-31G(d) basis set was used for the other atoms (GEN1). At the B3LYP/GEN1 level, frequency analysis was performed to ensure the stationary point as minimum or transition state. The IRC calculation<sup>4</sup> was applied for each transition state to confirm that it connects the right reactant and product. For the solvent effect, the single-point calculation on the gas-phase optimized geometry with SMD solvation model<sup>5</sup> (solvent = dichloroethane) was applied. The single-point calculation was carried out by using M06<sup>6</sup> with GEN2 (i.e., LANL2DZ with additional polarization function  $\zeta(f) = 1.350$  and  $\zeta(f) = 3.525$  for Rh and Cu<sup>7</sup>, respectively; 6-311+G(d,p) for the rest of atoms). Solution-phase single-point energy corrected by gas-phase Gibbs free energy correction was used for the reported energy in this study.

## References:

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**Table S1.** Thermal correction of Gibbs free energy (TCG, hartree) and total electronic energies (E, hartree) in dichloroethane solvent for all species involved in this study.

Compounds	TCG	E	Compounds	TCG	E
<b>Rh0</b>	0.225446	-727.714086044	<b>TS3</b>	0.623824	-1464.10202892
<b>2a</b>	0.413971	-965.383159813	<b>Int5</b>	0.625374	-1464.11656845
<b>Int1</b>	0.672715	-1693.14263146	<b>HOAc</b>	0.034692	-229.039342612
<b>TS1</b>	0.671216	-1693.11492873	<b>Cu(OAc)<sub>2</sub></b>	0.062638	-653.089850722
<b>Int2</b>	0.676464	-1693.13487902	<b>CuOAc</b>	0.018881	-424.655198463
<b>Int3</b>	0.621307	-1464.08215499	<b>1a</b>	0.29942	-807.102497848
<b>TS2</b>	0.620935	-1464.06714042	<b>isobutene</b>	0.081225	-157.135240434
<b>Int4</b>	0.624311	-1464.13123252			

**Cartesian coordinates for all optimized geometries**

**1a**

N	-1.64196100	1.09153100	0.10922200
N	1.25407800	-1.66284400	-0.80132500
C	-0.58019600	0.27049600	-0.19578700
C	-1.00995800	-1.06759900	-0.29461300
C	-2.43523500	-1.05422400	-0.01982500
C	-2.78440000	0.30565600	0.23439400
C	-4.09182600	0.68290700	0.54816200
H	-4.34957800	1.71841900	0.75081000
C	-5.06090400	-0.31876000	0.59834600
H	-6.08621400	-0.05218500	0.84016900
C	-4.73722800	-1.66261800	0.34593700
H	-5.51584700	-2.41850400	0.39412400
C	-3.43028600	-2.03610500	0.03782700
H	-3.18654600	-3.07774400	-0.15350500
C	-0.02001800	-2.00512900	-0.60790300
H	-0.25376600	-3.06475800	-0.70796500
C	1.03339800	2.15054200	-0.22830000
C	-1.46027000	2.52157900	0.30442700
C	-0.23485300	2.99183800	-0.50099900
H	1.39807400	2.35895400	0.78870500
H	1.82908100	2.47400100	-0.90807900
H	-2.36004300	3.04666000	-0.03445400
H	-1.32988000	2.74455000	1.37373500
H	-0.47875800	2.93498300	-1.56898600
H	-0.04454800	4.04520800	-0.26762300
C	0.74310900	0.67039800	-0.38666300
C	1.63735000	-0.36390600	-0.69571600
C	3.11862200	-0.12750200	-0.89389500
C	3.94223600	-0.47880400	0.36171100
H	3.31527900	0.91375000	-1.17766300
H	3.45327400	-0.76085900	-1.72397300
C	5.45311700	-0.31110600	0.15830900
H	3.61318200	0.14902400	1.20284200
H	3.71672700	-1.51575100	0.64245900
C	6.26949700	-0.66761000	1.40536300
H	5.77539000	-0.94047800	-0.68328800
H	5.66932300	0.72594400	-0.13726300
H	7.34430200	-0.54162100	1.23052300
H	5.99320700	-0.03144900	2.25553700

H 6.09958500 -1.70926400 1.70395200

**2a**

N	0.85451900	-1.71506400	-0.58831900
N	1.70526600	2.46815900	-0.12387600
C	0.86575300	-0.34391500	-0.48873300
C	2.13495200	0.11113400	-0.19119700
C	2.97344500	-1.06250600	-0.09676200
C	2.13925400	-2.18697500	-0.34712600
C	2.62965500	-3.49784700	-0.33887100
H	1.98257400	-4.34883600	-0.53204900
C	3.98352200	-3.67761000	-0.07418900
H	4.39544400	-4.68293600	-0.06059200
C	4.82807900	-2.57781200	0.17734400
H	5.88097800	-2.75211600	0.38185300
C	4.33695700	-1.27744100	0.16683200
H	5.00238700	-0.44019800	0.36052000
C	2.53425400	1.50101600	-0.01388000
H	3.59687300	1.65022200	0.22210400
C	2.11601900	3.86665700	0.06240700
C	1.76348600	4.59473400	-1.25164000
H	0.71177000	4.42861900	-1.50579700
H	1.93703800	5.67358300	-1.15905400
H	2.37547800	4.21728400	-2.07892700
C	3.60174700	4.09874800	0.39629000
H	4.26086100	3.72835100	-0.39794500
H	3.79333000	5.17140600	0.51028900
H	3.88916400	3.61088200	1.33534700
C	1.23895700	4.41954400	1.20531900
H	1.47067000	3.91300600	2.14932600
H	1.40584900	5.49484300	1.34123800
H	0.17991400	4.25345600	0.98378300
C	-1.48600800	-2.06888500	1.41369000
C	-0.32241300	-2.53644000	-0.84172600
C	-0.94953100	-3.13080100	0.42859300
H	-0.64900700	-1.45640500	1.77487800
H	-1.89039500	-2.58160800	2.29671000
H	-1.05730000	-1.90979200	-1.35532300
H	-0.03731000	-3.33996300	-1.53008400
H	-1.77044000	-3.79052300	0.12095900
H	-0.21056900	-3.75080600	0.94988300
C	-2.51319600	-1.20008000	0.83156300
C	-3.34591400	-0.48101200	0.32501000

C	-4.38250300	0.38111500	-0.24863400	O	-0.64589400	1.20192700	0.00000700
C	-5.81591900	-0.05634800	0.12188900	C	-0.09250500	0.12563700	-0.00004700
H	-4.28194300	0.40074700	-1.34349900	C	1.39758800	-0.10965900	0.00000700
H	-4.22158600	1.41617900	0.08565800	H	1.68543400	-0.69134700	-0.88202000
C	-6.88708300	0.86270900	-0.47739600	H	1.91744400	0.84858400	0.00014600
H	-5.97481400	-1.08734500	-0.22075400	H	1.68529300	-0.69148800	0.88199400
H	-5.91098400	-0.07597200	1.21546900	H	-1.72357900	-0.80313900	0.00011600
C	-8.31313500	0.43245000	-0.11763300				
H	-6.71623900	1.89230300	-0.13206900				
H	-6.77609100	0.88568700	-1.57098400				
H	-9.05628500	1.10727000	-0.55728700				
H	-8.52501800	-0.58024900	-0.48196500				
H	-8.46453200	0.43157900	0.96873900				
H	-0.04058400	0.22707600	-0.63197300				

### Cu(OAc)2

Cu	0.00000400	0.00030000	-0.00857100
O	1.67809200	-1.09013000	-0.00865000
O	1.67700300	1.09088900	-0.00891000
C	2.34168700	0.00078300	-0.00756600
C	3.84175200	0.00017300	0.02558100
H	4.23048600	-0.86697000	-0.51335000
H	4.23175500	0.92778800	-0.39831700
H	4.17281300	-0.07136100	1.06850100
O	-1.67845500	1.09061400	-0.00861000
C	-2.34167800	-0.00038700	-0.00766100
O	-1.67667700	-1.09041100	-0.00898700
C	-3.84172800	-0.00131900	0.02549100
H	-4.23173300	0.88831700	-0.47399200
H	-4.17257800	0.02030800	1.07076700
H	-4.23077700	-0.90997300	-0.43887500

### CuOAc

Cu	-1.30451300	-0.00043800	0.00380800
O	0.44668500	-1.11317200	-0.00914300
O	0.44437500	1.11433000	-0.00905700
C	1.06282900	0.00127000	-0.01480400
C	2.57897900	0.00087400	0.00557300
H	2.96550600	-0.86505400	-0.53633600
H	2.96852400	0.92804000	-0.41891100
H	2.91751500	-0.07243200	1.04580300

### HOAc

O	-0.77849200	-1.04673600	-0.00000600
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### Rh0

Rh	-0.36383800	0.00018000	-0.16320000
C	1.14583100	0.00157700	1.35798000
C	1.88622400	1.58563900	-1.99178700
H	2.97079400	1.68256200	-2.13934900
H	1.47444400	2.59048800	-1.87623100
H	1.47183000	1.14609200	-2.90324600
C	1.62047600	-0.73710600	-0.79149200
C	1.62140600	0.73340400	-0.79357200
C	1.88433600	-1.59320900	-1.98716700
H	2.96880800	-1.69354400	-2.13317600
H	1.47220600	-1.15495600	-2.90025900
H	1.46964700	-2.59661300	-1.86939100
C	0.87624200	0.00385300	2.82450000
H	1.83546500	0.00498600	3.36283600
H	0.32293300	-0.88411400	3.13917100
H	0.32249100	0.89255800	3.13632500
C	1.29815500	2.60012800	1.00859600
H	2.26465700	2.88640300	1.44409200
H	0.53396200	2.73349300	1.77879600
H	1.08003800	3.29332700	0.19344500
C	1.35864300	-1.18341900	0.53423100
C	1.36022500	1.18382600	0.53089200
C	1.29507900	-2.59823200	1.01607800
H	2.26086000	-2.88379300	1.45364100
H	1.07755300	-3.29371500	0.20271900
H	0.52983900	-2.72882500	1.78571900
C	-2.84139100	0.00179300	-0.16188200
O	-2.16646400	-1.09141000	-0.11892100
O	-2.16641200	1.09431800	-0.11996900
C	-4.32765600	0.00005500	-0.28336900
H	-4.59711900	-0.09140700	-1.34312200
H	-4.74691400	-0.85942000	0.24546400
H	-4.74122000	0.93526500	0.09962100

### Int1

N	0.82489000	2.85431200	-0.66350900	C	7.48748800	-2.24499600	-0.05389700
N	-1.85536100	-0.09269900	1.49831900	H	7.42175100	-0.08029500	0.05730500
C	0.35426200	1.72951800	-0.05346500	H	6.66068600	-0.88636500	1.42080300
C	-0.84292700	2.00411200	0.60467800	C	8.85477100	-2.41105900	0.61748000
C	-1.10875800	3.41599600	0.38702900	H	6.84149100	-3.09362900	0.21435100
C	-0.05662100	3.90965300	-0.42207800	H	7.60730900	-2.28541800	-1.14593100
C	-0.00679700	5.23805900	-0.85741900	H	9.32853600	-3.35427800	0.32480600
H	0.80139400	5.60534900	-1.48213000	H	9.53406000	-1.59639600	0.33967500
C	-1.03871500	6.08087400	-0.45765000	H	8.76298700	-2.40830200	1.71027800
H	-1.03077700	7.11940200	-0.77419900	Rh	-1.37575600	-1.36139900	-0.23143800
C	-2.09346500	5.61105400	0.34918700	C	-2.94709300	-2.44854000	-1.36043200
H	-2.88193500	6.29672300	0.64465000	C	0.10273800	-1.11686100	-3.16429300
C	-2.14383200	4.28600700	0.76727500	H	-0.06180800	-1.19924600	-4.24696500
H	-2.97284800	3.93769400	1.37792600	H	0.87766400	-1.83452100	-2.88548400
C	-1.62637300	1.18615200	1.49265400	H	0.48047300	-0.11232600	-2.96047100
H	-2.09239500	1.77210600	2.28625300	C	-2.14812000	-0.37133300	-2.04988000
C	-2.54377400	-0.66108400	2.72907000	C	-1.17841200	-1.37885300	-2.43875000
C	-3.30714000	-1.93849100	2.35309000	C	-2.13875400	1.06969200	-2.45560000
H	-2.64863000	-2.68281200	1.90261900	H	-2.69185200	1.18781100	-3.39771600
H	-3.73889200	-2.37896600	3.25765300	H	-1.12571700	1.44311000	-2.61586800
H	-4.13284700	-1.71681500	1.66978100	H	-2.61269000	1.70751200	-1.70634100
C	-3.55582500	0.32376100	3.35685000	C	-3.81716400	-3.55255600	-0.84840800
H	-4.25538300	0.71479400	2.60926100	H	-4.27816600	-4.07649600	-1.69657800
H	-4.13937600	-0.21341800	4.11026000	H	-4.62030600	-3.18341800	-0.20836000
H	-3.08409600	1.16596100	3.87257100	H	-3.23900200	-4.28985100	-0.28346700
C	-1.44823200	-0.99865600	3.76078000	C	-0.99647800	-3.98568000	-2.19730400
H	-0.86363100	-0.10811200	4.01692700	H	-1.48187700	-4.52074400	-3.02404800
H	-1.90812200	-1.37852700	4.67965400	H	-1.07774800	-4.60884000	-1.30218500
H	-0.77480100	-1.76795400	3.37636300	H	0.06285200	-3.88476700	-2.44455600
C	3.64135700	2.81239700	0.73305900	C	-3.25461200	-1.05158100	-1.41516300
C	2.11733600	2.97761200	-1.34392600	C	-1.64876400	-2.65271500	-1.99276900
C	3.20089800	3.64886700	-0.48798900	C	-4.52845000	-0.39082700	-0.98804600
H	2.78437100	2.65987100	1.40375500	H	-5.16037900	-0.21575700	-1.86887800
H	4.37023000	3.39767000	1.30882600	H	-4.34250500	0.57931500	-0.51992700
H	2.43896600	1.97025200	-1.62333300	H	-5.09945200	-1.00617000	-0.29020600
H	1.95629600	3.54555800	-2.26634000	C	0.68211300	-2.26998300	1.02055700
H	4.06822200	3.82708600	-1.13420200	O	-0.44188300	-2.85714000	1.11965800
H	2.84772800	4.62710200	-0.14242400	O	0.75099100	-1.24397900	0.26335400
C	4.23134500	1.52260300	0.36289800	H	0.93233500	0.81653200	-0.05941100
C	4.73494200	0.47476400	0.02224000	C	1.88122300	-2.73834300	1.79491000
C	5.41069800	-0.77313300	-0.34444800	H	2.80238300	-2.45938400	1.27868400
C	6.79011000	-0.93472600	0.33180400	H	1.88241200	-2.25242400	2.77811400
H	5.53534900	-0.81723000	-1.43597800	H	1.83739500	-3.81885700	1.94950600
H	4.77595000	-1.63213700	-0.08033200				

## Int2

N	-0.59415200	2.23341600	-0.71638400	H	5.25775600	0.01443900	2.16782400
N	-2.42990500	-0.96085300	0.97644700	C	7.27368500	-0.42797900	0.31032300
C	-1.09166900	1.04070900	-0.25228800	H	5.78803900	0.72252300	-0.77324900
C	-2.37962700	1.28103400	0.26286800	H	6.47596700	1.56645900	0.60643700
C	-2.71284700	2.66955500	0.05316600	C	8.47342300	-0.00812300	-0.54523200
C	-1.57883100	3.23581700	-0.58080700	H	7.59575300	-0.56221800	1.35250700
C	-1.55865300	4.57195600	-0.99527500	H	6.90814100	-1.40942200	-0.02508700
H	-0.70931900	5.00060900	-1.51627400	H	9.27714200	-0.75005600	-0.49066400
C	-2.68918400	5.34464100	-0.73984200	H	8.19164300	0.10161200	-1.59952600
H	-2.70349800	6.38339100	-1.05555700	H	8.88290400	0.95186900	-0.20929800
C	-3.81149600	4.80323500	-0.08773900	Rh	-0.62845100	-0.96239800	-0.34157100
H	-4.67522800	5.43420800	0.09899400	C	0.49658500	-2.77818500	-1.32427400
C	-3.83563700	3.46999600	0.30782900	C	-0.29495000	0.23118100	-3.49797700
H	-4.71544000	3.05725500	0.79382300	H	-0.36556000	-0.15325600	-4.52423100
C	-3.01969600	0.20334500	0.92892900	H	0.60349800	0.84642100	-3.44114100
H	-3.96216200	0.36851400	1.45216400	H	-1.16448100	0.87052300	-3.32655200
C	-3.01509200	-2.03164700	1.85155900	C	-1.37952800	-1.77214100	-2.23732900
C	-1.97232200	-3.14169400	2.03855400	C	-0.25027500	-0.92902900	-2.55115400
H	-1.08291100	-2.76575100	2.55286600	C	-2.76069000	-1.62185600	-2.80141200
H	-2.39594100	-3.95149700	2.64131800	H	-2.82990300	-2.13205900	-3.77218300
H	-1.65705200	-3.55969800	1.08211600	H	-3.02060700	-0.57206500	-2.95828500
C	-4.28767300	-2.59365500	1.18767700	H	-3.51452200	-2.06158000	-2.14348800
H	-4.07213300	-2.99784900	0.19393300	C	1.44668400	-3.69584000	-0.62001600
H	-4.71335400	-3.39824200	1.79686700	H	2.18409300	-4.09999200	-1.32573800
H	-5.05274200	-1.81751600	1.07547500	H	0.93228700	-4.53923900	-0.15387700
C	-3.36107800	-1.46420800	3.24708200	H	1.99735000	-3.15940900	0.16036000
H	-4.19117500	-0.75128300	3.21966900	C	2.31236400	-1.00718200	-1.96090000
H	-3.66086800	-2.28048600	3.91216700	H	2.91257800	-1.70610500	-2.55817600
H	-2.49362700	-0.96338700	3.69027300	H	2.76466800	-0.94326300	-0.96674100
C	1.94648500	3.04101300	1.08163400	H	2.39266700	-0.02406500	-2.42940000
C	0.76841200	2.50611200	-1.18440000	C	-0.86762700	-2.97952300	-1.58250600
C	1.55692300	3.51699000	-0.33272900	C	0.89039700	-1.47917800	-1.88728400
H	1.04841600	2.73499700	1.63237600	C	-1.65613100	-4.23865600	-1.38701500
H	2.34930800	3.90272700	1.63024500	H	-1.73588200	-4.76248700	-2.34957500
H	1.29503800	1.55077300	-1.19888600	H	-2.67479400	-4.04535700	-1.04368100
H	0.71040200	2.88171800	-2.21326200	H	-1.17994400	-4.92392800	-0.68237000
H	2.46892600	3.76180300	-0.88979600	C	0.70222700	-0.31302100	2.46851000
H	0.98894900	4.44585600	-0.23424400	O	0.69746400	-1.00590700	1.44416900
C	2.94579000	1.96690600	1.09584300	O	-0.11933900	0.70659700	2.65949400
C	3.81707000	1.12351400	1.11053500	H	-0.67069500	0.84426100	1.85157100
C	4.92002500	0.15622100	1.13122600	C	1.65022600	-0.55115100	3.60545800
C	6.12372800	0.58548900	0.26342400	H	2.43764200	0.20916900	3.55462200
H	4.56396900	-0.82913200	0.79576800	H	1.13345300	-0.44205900	4.56258500
				H	2.09885200	-1.54111700	3.51965800

**Int3**

N	-2.36809000	0.98113800	-0.92153800
N	-0.19053100	-0.94692600	1.81794800
C	-1.57580700	0.17909600	-0.15394600
C	-2.26709500	-0.19093300	0.99954100
C	-3.59091300	0.39555600	0.93100400
C	-3.61499700	1.14109800	-0.27723000
C	-4.73305700	1.87110900	-0.68192400
H	-4.74277100	2.43920800	-1.60749800
C	-5.85093900	1.84810800	0.15080300
H	-6.73790400	2.40574500	-0.13401600
C	-5.84836500	1.11401600	1.34963900
H	-6.73641600	1.11361500	1.97459400
C	-4.72994500	0.38569800	1.74745200
H	-4.74609600	-0.18076700	2.67449800
C	-1.46550400	-0.73738500	2.03046500
H	-1.88838400	-0.89739400	3.02160700
C	0.68662600	-1.19460700	3.01213500
C	2.02067300	-1.79612900	2.55948200
H	2.44594100	-1.24016100	1.72053700
H	2.73850400	-1.77653400	3.38609700
H	1.89613900	-2.83751600	2.25637300
C	0.03838100	-2.18374900	4.00679900
H	-0.27126700	-3.10456100	3.50036700
H	0.77034300	-2.45022500	4.77616100
H	-0.82802900	-1.76478100	4.52732900
C	0.92857400	0.16095400	3.71008800
H	-0.01365100	0.58710500	4.07167000
H	1.59578000	0.03620700	4.56997200
H	1.37973600	0.88236400	3.02231600
C	-0.41998200	2.89436900	-0.05073600
C	-1.83635200	1.86602100	-1.95073800
C	-1.20365100	3.13819900	-1.35699600
H	-1.12815700	2.66978800	0.75522700
H	0.07862900	3.83036400	0.23410500
H	-1.07799700	1.30392800	-2.49327100
H	-2.63092600	2.12012400	-2.65766400
H	-0.55262500	3.58770600	-2.11609600
H	-1.98211100	3.87377400	-1.12766700
C	0.63122500	1.85184800	-0.04789800
C	1.70970700	1.28817500	0.18438000
C	3.14273800	1.21650400	0.55122600
C	3.84056200	2.58458000	0.38082800
H	3.66461700	0.46181300	-0.04438600

H	3.22574500	0.89020200	1.59541700
C	5.31981500	2.53785800	0.78708900
H	3.75081900	2.90571200	-0.66527100
H	3.31336200	3.33409400	0.98503400
C	6.02146100	3.88926900	0.61571900
H	5.39930200	2.21249200	1.83367200
H	5.83795300	1.77583200	0.18782000
H	7.07345600	3.82575800	0.91238700
H	5.98871100	4.22508500	-0.42758400
H	5.54796000	4.66344700	1.23086400
Rh	0.30372300	-0.52701700	-0.33180400
C	1.96490300	-1.57506300	-1.75665700
C	-1.61081900	-1.47054000	-3.01111000
H	-1.67346300	-2.30552300	-3.72173800
H	-1.67745600	-0.54797500	-3.59041100
H	-2.48385700	-1.52840500	-2.35744100
C	-0.07023000	-2.53821600	-1.20212900
C	-0.32175200	-1.58482500	-2.25307400
C	-1.05996200	-3.53229000	-0.67135500
H	-1.08883900	-4.42652600	-1.30874800
H	-2.06794700	-3.11158900	-0.63747900
H	-0.79975700	-3.85348000	0.34035900
C	3.43105900	-1.33852300	-1.95609200
H	3.79006800	-1.93220500	-2.80841400
H	4.02076500	-1.63775200	-1.08505100
H	3.65125000	-0.29205600	-2.18335400
C	1.17844700	0.12232800	-3.57555400
H	1.74794400	-0.33602700	-4.39476600
H	1.77015700	0.96164100	-3.19626600
H	0.25931100	0.52375200	-4.00809700
C	1.37699500	-2.59360000	-0.99171000
C	0.90614400	-0.89338500	-2.50427300
C	2.09658700	-3.68399100	-0.25860200
H	2.32336800	-4.49635300	-0.96342100
H	1.48913800	-4.11432800	0.53979700
H	3.04429400	-3.34860900	0.16901700

**Int4**

N	-3.07114000	1.29663700	-0.65051900
N	0.17505900	-0.71786800	1.62889200
C	-1.84586000	0.95838400	-0.11652800
C	-2.03540100	-0.14806600	0.74329900
C	-3.44468900	-0.47860600	0.71111000
C	-4.05707600	0.43601200	-0.17462700



C	-5.42600500	0.40996700	-0.45350100	H	3.17033400	-4.02080000	0.13781400
H	-5.88569200	1.11941700	-1.13428400	H	4.22249900	-2.59839600	0.09325700
C	-6.18777800	-0.56664200	0.18266700	C	1.20273100	0.35436300	-3.42519900
H	-7.25544400	-0.61703400	-0.00777800	H	1.16611000	-0.06805800	-4.43784800
C	-5.59757300	-1.49026600	1.06600400	H	2.00676200	1.09433100	-3.40538300
H	-6.22021600	-2.24027900	1.54445900	H	0.25953700	0.87713600	-3.24693300
C	-4.23201600	-1.46100000	1.33134300	C	-1.02887200	-1.65506500	-2.30384900
H	-3.79087300	-2.18940000	2.00676200	H	-1.13491900	-2.29523300	-3.19184000
C	-1.12243200	-0.67582500	1.70247700	H	-1.39667600	-0.65990000	-2.56263200
H	-1.59266600	-1.06592200	2.60889100	H	-1.67362300	-2.06175200	-1.52115300
C	0.96902700	-1.12419000	2.84284500	C	2.65215600	-1.14729400	-1.84793700
C	2.40003200	-0.59230000	2.65011300	C	0.40571100	-1.62221500	-1.88317400
H	2.40959200	0.50172600	2.60637200	C	4.00207400	-0.53810400	-2.07081400
H	3.03866900	-0.90217200	3.48398200	H	4.55392600	-1.11466900	-2.82587600
H	2.85496500	-0.98690700	1.73006100	H	4.60499500	-0.54721700	-1.15691200
C	0.98228000	-2.65984800	2.95170600	H	3.93384900	0.49267400	-2.42597300
H	1.42507500	-3.11623800	2.06106000	C	1.79266000	2.33672200	-0.31657900
H	1.56960300	-2.97258500	3.82162900	C	1.94093200	3.25643200	0.91671400
H	-0.03250000	-3.05467800	3.07197400	H	1.73431000	2.95915900	-1.22314900
C	0.39253300	-0.50158100	4.12987400	H	2.72444100	1.76412100	-0.42139400
H	-0.57432200	-0.92938800	4.41145000	C	3.17572300	4.16390000	0.83447200
H	1.07883700	-0.68917000	4.96209100	H	1.03938500	3.87116000	1.02932100
H	0.27478600	0.58186800	4.02207700	H	1.99905100	2.63753000	1.82254700
C	-1.06923400	3.24897800	-0.71470300	C	3.32572100	5.07945400	2.05420500
C	-3.36982600	2.49926600	-1.43104300	H	4.07694500	3.54299100	0.72793800
C	-2.09048900	3.21205200	-1.86314800	H	3.11665600	4.77446500	-0.07761500
H	-1.50661200	3.77576400	0.14594900	H	4.21418300	5.71352900	1.96605000
H	-0.19305900	3.82161300	-1.02368600	H	2.45625500	5.73826100	2.16536900
H	-3.97340000	2.21264500	-2.29921100	H	3.42229300	4.49756600	2.97888600
H	-3.98497100	3.16211300	-0.80824100				
H	-1.64720000	2.70063500	-2.72697400	<b>Int5</b>			
H	-2.34851400	4.22553200	-2.18818300	N	-3.22618500	0.59301400	-1.07579000
C	-0.68531400	1.82105600	-0.33154100	N	0.19992800	0.51270800	1.33242000
C	0.59985500	1.39256400	-0.25529800	C	-2.01198100	0.63545700	-0.42629700
Rh	1.20615500	-0.54368100	-0.20964400	C	-2.10816700	-0.09021300	0.80648500
C	1.42611900	-0.73780100	-2.42249700	C	-3.47366000	-0.60031600	0.87387500
C	0.37205100	-3.91954300	-0.61552300	C	-4.13151500	-0.13228400	-0.29629100
H	0.00989800	-4.55335900	-1.43548000	C	-5.47582600	-0.41274400	-0.53658400
H	-0.50094100	-3.62722600	-0.02297500	H	-5.98439700	-0.04560600	-1.42233600
H	1.02093000	-4.53194900	0.01460900	C	-6.15511400	-1.18416100	0.40929800
C	2.44254600	-2.42354300	-1.12102700	H	-7.20289200	-1.41725700	0.24404700
C	1.08644100	-2.72319400	-1.16429200	C	-5.51835300	-1.65999200	1.56522300
C	3.55055300	-3.22330500	-0.50514700	H	-6.07724500	-2.25555500	2.27998000
H	4.16388400	-3.69223500	-1.28608200	C	-4.17516100	-1.36847500	1.80501400

H	-3.68789400	-1.73284700	2.70570100	H	-0.71329100	-3.76012500	-1.71091700
C	-1.03073400	-0.12809500	1.62710600	H	-1.18994700	-2.05914100	-1.79527200
H	-1.07062200	-0.63322100	2.57690100	H	-1.18062900	-2.90084800	-0.23869000
C	0.92833200	0.91566400	2.66574800	C	2.90755300	-1.67926900	-1.39779500
C	2.36905100	1.40442800	2.44242700	C	0.78260500	-2.41362200	-0.99744400
H	2.43340500	2.40079600	2.01092500	C	4.12684900	-1.05211100	-2.00462800
H	2.86111500	1.45117300	3.41799800	H	4.73353600	-1.81226300	-2.51606100
H	2.94515500	0.69837700	1.82815300	H	4.76648800	-0.59203000	-1.24422300
C	1.04827700	-0.34388000	3.55830600	H	3.86727200	-0.28619800	-2.74035400
H	1.47133000	-1.18439700	2.99851600	C	1.36389400	2.26622400	-0.29472000
H	1.72516200	-0.11434100	4.38563700	C	1.01982800	3.70838500	0.14688500
H	0.10785400	-0.65706100	4.01669100	H	1.46472800	2.27416400	-1.38379300
C	0.09083000	1.99112600	3.37563400	H	2.36019900	2.00011700	0.06544200
H	-0.90704500	1.61958500	3.62725500	C	1.98762300	4.74026300	-0.45082800
H	0.58527600	2.28207700	4.30855300	H	-0.00753500	3.94469000	-0.15790900
H	-0.02551600	2.88696100	2.76105600	H	1.03696100	3.79485000	1.23895300
C	-0.94312900	1.99021900	-2.17439800	C	1.67070500	6.17595300	-0.01942700
C	-3.44156700	1.35209200	-2.29770600	H	3.01647300	4.48710600	-0.15688400
C	-2.10438500	1.46103100	-3.04786900	H	1.95866400	4.67065000	-1.54723600
H	-1.06131000	3.07216200	-2.02203300	H	2.37534200	6.88537400	-0.46553900
H	-0.01323400	1.86445300	-2.74016300	H	0.66081700	6.47053700	-0.32889800
H	-4.18255600	0.83679100	-2.91669300	H	1.73097300	6.28769000	1.06974100
H	-3.84066800	2.34840600	-2.05903800				
H	-1.84186500	0.46713400	-3.43098100	TS1			
H	-2.23525100	2.11413700	-3.91633100	N	-0.42731900	2.32360100	-0.29876700
C	-0.87407300	1.26588400	-0.83861300	N	-2.18168500	-0.95579200	1.41122200
C	0.32347600	1.17340500	-0.01251300	C	-0.79386200	1.13148800	0.31270200
Rh	1.48374900	-0.59899700	-0.05050900	C	-2.08168100	1.32915500	0.86274700
C	1.61985900	-1.76564300	-1.98477600	C	-2.50632600	2.66487200	0.59378500
C	1.16469900	-3.86970700	1.16474500	C	-1.44050900	3.25906000	-0.14536500
H	0.91910600	-4.86489500	0.77044200	C	-1.51001700	4.58856200	-0.59414600
H	0.25430300	-3.47939500	1.63321600	H	-0.70090200	5.04536700	-1.15426800
H	1.91644100	-4.00272900	1.94731300	C	-2.66285300	5.30322500	-0.30253800
C	2.93924700	-2.50714300	-0.16380900	H	-2.74991900	6.33064800	-0.64304100
C	1.65240600	-2.97145100	0.06894000	C	-3.72944000	4.72701100	0.42680300
C	4.18084800	-2.77201900	0.63402700	H	-4.61102600	5.32502100	0.63601500
H	4.84585100	-3.46422900	0.10009000	C	-3.66401400	3.41831000	0.87410000
H	3.95277800	-3.21764500	1.60576400	H	-4.48877200	2.98279100	1.43105500
H	4.75455000	-1.85563900	0.81110300	C	-2.66316600	0.23730800	1.58553200
C	1.19475000	-1.29643000	-3.34426600	H	-3.44801300	0.42579100	2.32065000

H	-1.98302300	-3.67808200	1.04581500	H	-4.31714800	-1.13898400	-1.31058700
C	-4.08927400	-2.33953100	2.22317300	C	0.44366500	-3.74588800	-1.70881300
H	-4.33917800	-2.64386300	1.20136300	H	0.90566600	-4.05673200	-2.65421400
H	-4.37629500	-3.15353000	2.89680700	H	-0.09744200	-4.60199800	-1.30034700
H	-4.70273600	-1.46889100	2.47836600	H	1.24651500	-3.48743500	-1.01013400
C	-2.25756200	-1.59778000	3.80783600	C	1.40871600	-0.96352300	-2.81774900
H	-2.86914100	-0.74635800	4.12351600	H	1.59662100	-1.37525700	-3.81858500
H	-2.45249000	-2.41987500	4.50410200	H	2.13738900	-1.40709900	-2.13358500
H	-1.20452100	-1.31210600	3.89619700	H	1.59973000	0.11099000	-2.86168500
C	2.56823200	2.84909200	1.07122300	C	-1.86480800	-2.50660100	-1.75315100
C	0.87679800	2.63141200	-0.89433500	C	0.00510300	-1.26531600	-2.38617100
C	1.78081900	3.55457300	-0.05485800	C	-2.78978500	-3.64978000	-1.47128100
H	1.88149300	2.38235900	1.78655400	H	-3.23185200	-3.99041800	-2.41787100
H	3.12118500	3.61494600	1.63107100	H	-3.61474400	-3.36145700	-0.81578200
H	1.38451400	1.68039700	-1.07503700	H	-2.27495600	-4.50276900	-1.02538400
H	0.68713600	3.09867100	-1.86756300	C	1.33510500	-0.92389500	1.72608300
H	2.49757000	4.01984400	-0.74158300	O	0.83010600	-1.62105800	0.79407800
H	1.18322700	4.36425100	0.37811900	O	0.89641900	0.22304200	2.06701700
C	3.51039100	1.84503500	0.56562500	H	0.08404600	0.61908700	1.17302100
C	4.30028800	1.04178400	0.11723800	C	2.52519400	-1.46699000	2.47947400
C	5.32047800	0.11326900	-0.38203500	H	3.38057200	-0.81102100	2.28637700
C	6.69274300	0.29892700	0.30331800	H	2.32414800	-1.43781900	3.55475000
H	5.43860400	0.24704600	-1.46697600	H	2.75480400	-2.48672700	2.16775200
H	4.98408800	-0.92443600	-0.24059200				
C	7.75262000	-0.67578100	-0.22400500	TS2			
H	7.02740500	1.33312800	0.15262500	N	-2.37439200	0.65778000	-1.05940200
H	6.57130000	0.16828800	1.38662500	N	0.10709400	-0.50823600	1.96842100
C	9.11498300	-0.49637900	0.45408200	C	-1.39307700	0.28410200	-0.16314200
H	7.40280100	-1.70790400	-0.07758900	C	-1.96609500	0.21730400	1.11443300
H	7.86194900	-0.54097200	-1.30952200	C	-3.35856800	0.56899200	1.00806000
H	9.85096800	-1.20478900	0.05887000	C	-3.57799800	0.85814000	-0.36484800
H	9.50684200	0.51524800	0.29485400	C	-4.82731400	1.25813100	-0.84895800
H	9.04373500	-0.65823900	1.53639100	H	-4.99184400	1.48048700	-1.89885200
Rh	-0.85748600	-0.98225000	-0.37789400	C	-5.86822000	1.35878500	0.06899900
C	-0.45415400	-2.57001100	-1.93297300	H	-6.85108400	1.66714100	-0.27406100
C	-1.20089200	0.92755800	-3.17742400	C	-5.67224700	1.06463600	1.43310100
H	-1.55848900	0.82102600	-4.21063000	H	-6.50894400	1.14988200	2.11982300
H	-0.21567500	1.39364000	-3.21847800	C	-4.42993700	0.66652100	1.91114000
H	-1.88568900	1.60476300	-2.66078200	H	-4.29308400	0.43907900	2.96456900
C	-2.29774400	-1.15022400	-2.06096800	C	-1.11265500	-0.10856700	2.19674100

H	3.05549700	-1.19615000	3.58061400	H	-1.05446700	-3.84320400	0.73143700
H	2.22976300	-2.26515100	2.44473200	H	0.54591700	-3.85876800	1.48021200
C	0.38372000	-1.55180500	4.23046200	C	3.19373100	-1.10879700	-2.37981900
H	0.13238200	-2.52540000	3.79621200	H	3.57567500	-1.77239900	-3.16791500
H	1.09881800	-1.71566700	5.04329800	H	3.99066100	-0.99079500	-1.64061900
H	-0.52253500	-1.13300900	4.67882400	H	3.00522100	-0.13524100	-2.84186900
C	1.24451400	0.78291700	3.76301200	C	0.34744500	-1.03374300	-3.70744100
H	0.30882500	1.23569000	4.10742200	H	0.83344400	-1.65899300	-4.46885600
H	1.92166100	0.72206600	4.62173700	H	0.74224900	-0.01986700	-3.82780800
H	1.69089900	1.45416200	3.02247300	H	-0.71948100	-1.02463500	-3.93985800
C	-0.74478000	2.83799900	-0.80382300	C	1.88868000	-2.52601200	-0.63596000
C	-2.05704300	1.27498700	-2.34014900	C	0.62654200	-1.60154500	-2.34593300
C	-1.48336700	2.69833800	-2.15036600	C	3.08199100	-3.09924500	0.07329800
H	-1.47747000	3.00705700	-0.00629900	H	3.59424900	-3.80112100	-0.59872200
H	-0.09019400	3.71805000	-0.83035200	H	2.80243600	-3.65881100	0.96689600
H	-1.31916200	0.64395400	-2.83067200	H	3.80971100	-2.33651700	0.36351500
H	-2.95128400	1.28271000	-2.96712200				
H	-0.81092000	2.92308900	-2.98586600	<b>TS3</b>			
H	-2.28599900	3.44236600	-2.17196700	N	-3.18845900	0.69522400	-1.04607700
C	0.12674200	1.68920300	-0.41651500	N	0.26921500	0.37300100	1.42002200
C	1.28786900	1.24728000	-0.14488400	C	-1.94043600	0.64961600	-0.46348400
C	2.70184600	1.66817100	0.06791600	C	-2.03334900	-0.07497000	0.76536400
C	2.93662600	3.18074200	-0.11557000	C	-3.42251700	-0.49464700	0.89737500
H	3.34943000	1.10917900	-0.61905200	C	-4.10268300	0.01434700	-0.23696400
H	3.01457800	1.36931300	1.07651500	C	-5.47010200	-0.18415700	-0.42632000
C	4.40204400	3.57306600	0.11763300	H	-5.99054500	0.21618500	-1.29059200
H	2.63376600	3.47498200	-1.12985600	C	-6.15473000	-0.91674600	0.54481600
H	2.29187000	3.73470000	0.57994800	H	-7.22050000	-1.08696000	0.42492100
C	4.65227900	5.07439100	-0.05876200	C	-5.49550200	-1.43612200	1.67009300
H	4.70169600	3.26726600	1.12984100	H	-6.05777200	-2.00234400	2.40603900
H	5.04236000	3.00945200	-0.57545100	C	-4.12810100	-1.23115900	1.85286300
H	5.70489800	5.32049200	0.11534400	H	-3.62556000	-1.63801900	2.72662100
H	4.39680300	5.40439200	-1.07285500	C	-1.00237100	-0.07344700	1.67122300
H	4.05209200	5.66298800	0.64524100	H	-1.21724500	-0.37124800	2.69167500
Rh	0.45022700	-0.70442400	-0.27805800	C	1.07289900	0.64529200	2.70392500
C	1.95266800	-1.69304000	-1.77503100	C	2.50593900	1.08911800	2.37422900
C	-1.68206500	-2.78465400	-1.90598200	H	2.55341100	2.09642400	1.96120900
H	-1.72887400	-3.64241400	-2.58976700	H	3.09603800	1.08759200	3.29568600
H	-2.19233300	-1.94737000	-2.38824200	H	2.99825900	0.39108500	1.68113300
H	-2.25120700	-3.04474100	-1.00980100	C	1.18035200	-0.67012000	3.50847800
C	0.49772600	-2.97484000	-0.48893700	H	1.62191700	-1.46361700	2.89657700
C	-0.25481300	-2.45981900	-1.57771800	H	1.82812100	-0.50638600	4.37558800
C	0.01354400	-3.96124600	0.53141900	H	0.21925800	-1.02332000	3.89094300
H	0.17329900	-4.98697900	0.17225400	C	0.37476700	1.73568600	3.53497400

H	-0.61891000	1.42433900	3.87087300	C	2.42101900	4.59533600	-0.20454000
H	0.96944200	1.95868300	4.42723600	H	0.33370700	4.02920100	-0.29527900
H	0.26282100	2.65998600	2.96080600	H	1.12908500	3.56628200	1.19279700
C	-1.09320600	2.38487300	-1.99702500	C	2.19023200	5.99950700	0.36385700
C	-3.49196500	1.52867700	-2.20306100	H	3.35965600	4.18653100	0.19709600
C	-2.19454200	1.86993400	-2.94516800	H	2.55808800	4.65680200	-1.29330400
H	-1.40596900	3.35010400	-1.57411000	H	3.02670000	6.66389400	0.12358800
H	-0.18809400	2.58223500	-2.57935600	H	1.27869700	6.44983200	-0.04667000
H	-4.17944500	0.98881600	-2.86319300	H	2.08717100	5.97528600	1.45532500
H	-4.00254500	2.44364700	-1.87127200				
H	-1.83347000	0.97712200	-3.47033000	<b>isobutene</b>			
H	-2.41313200	2.62448900	-3.70746800	C	1.27840700	-0.67917300	-0.00000300
C	-0.83263200	1.37441600	-0.88309500	C	-0.00000400	0.12277300	0.00000200
C	0.43060000	1.17056600	-0.27618200	H	1.33328500	-1.33419400	-0.88079900
Rh	1.38848500	-0.62995300	-0.10193600	H	2.16342400	-0.03543000	0.00130100
C	1.43809400	-1.74793300	-2.05953100	H	1.33206900	-1.33619000	0.87937500
C	0.95347800	-3.89320500	1.05603900	C	0.00019800	1.45970700	-0.00000800
H	0.65005100	-4.86723300	0.64997800	C	-1.27858400	-0.67883300	-0.00000200
H	0.07606400	-3.46414600	1.55196400	H	-0.92432400	2.03209500	-0.00018000
H	1.71585000	-4.07707500	1.81741800	H	0.92512000	2.03149300	0.00020100
C	2.75969300	-2.58994000	-0.29222000	H	-1.33348000	-1.33418700	0.88056500
C	1.45782700	-3.00106300	-0.03712100	H	-2.16344400	-0.03486500	-0.00082500
C	4.00448300	-2.92394900	0.47341000	H	-1.33275000	-1.33556100	-0.87956900
H	4.62191900	-3.63894400	-0.08674400				
H	3.77835600	-3.37250200	1.44398700				
H	4.62482700	-2.03802600	0.64736400				
C	0.98747800	-1.20623400	-3.38272600				
H	0.87283900	-2.01849700	-4.11285800				
H	1.70751400	-0.49457500	-3.79553000				
H	0.02061400	-0.69943500	-3.30216300				
C	-0.85801000	-2.71273200	-1.24748000				
H	-0.95487800	-3.67936600	-1.76289700				
H	-1.37243200	-1.96296900	-1.85311600				
H	-1.38055900	-2.79588200	-0.29145200				
C	2.74327800	-1.74588600	-1.51447300				
C	0.59095300	-2.38716800	-1.06956500				
C	3.97856900	-1.16831800	-2.13719000				
H	4.55226200	-1.95529300	-2.64571300				
H	4.64090700	-0.72500700	-1.38623500				
H	3.74124900	-0.40012100	-2.87757900				
C	1.51942500	2.21772200	-0.47036600				
C	1.27066600	3.62742400	0.10730600				
H	1.64132200	2.30212300	-1.55972500				
H	2.49019100	1.85233400	-0.11836800				